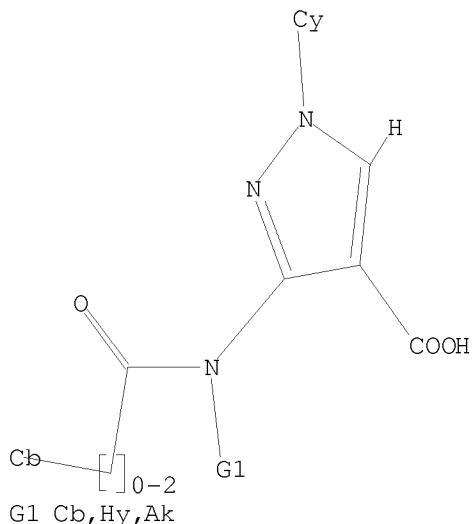


L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

FULL SEARCH INITIATED 14:58:35 FILE 'REGISTRY'
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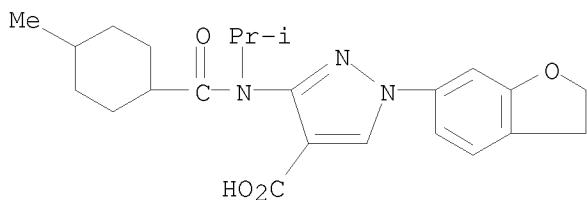
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331 ANSWERS

L2 331 SEA SSS FUL L1

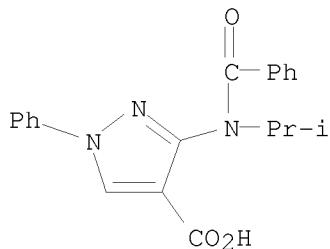
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L2 ANSWER 1 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
RN 1026248-17-8 REGISTRY
ED Entered STN: 08 Jun 2008
CN INDEX NAME NOT YET ASSIGNED
MF C23 H29 N3 O4
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)



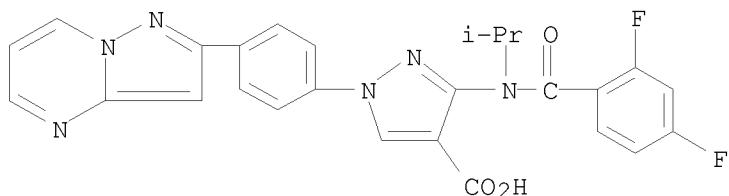
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 2 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
RN 1026009-81-3 REGISTRY
ED Entered STN: 06 Jun 2008
CN 1H-Pyrazole-4-carboxylic acid, 3-[benzoyl(1-methylethyl)amino]-1-phenyl- (CA INDEX NAME)
MF C20 H19 N3 O3
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 3 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
RN 934333-11-6 REGISTRY
ED Entered STN: 06 May 2007
CN 1H-Pyrazole-4-carboxylic acid, 3-[(2,4-difluorobenzoyl)(1-methylethyl)amino]-1-(4-pyrazolo[1,5-a]pyrimidin-2-ylphenyl)- (CA INDEX NAME)
OTHER NAMES:
CN 3-[(2,4-Difluorophenyl)carbonyl](1-methylethyl)amino]-1-[4-(pyrazolo[1,5-a]pyrimidin-2-yl)phenyl]-1H-pyrazole-4-carboxylic acid
MF C26 H20 F2 N6 O3
SR CA
LC STN Files: CA, CAPLUS



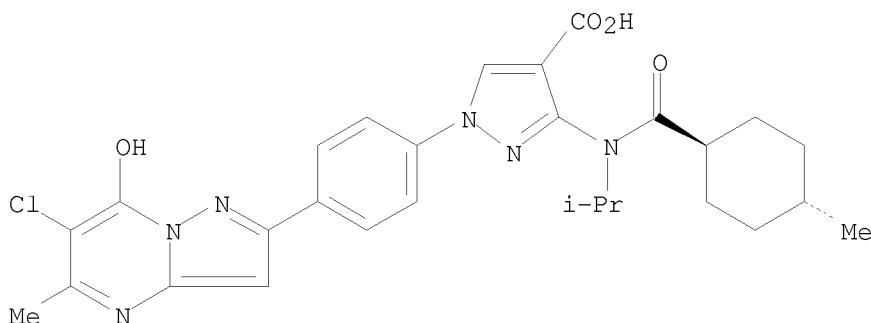
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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 4 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN

RN 934333-10-5 REGISTRY
 ED Entered STN: 06 May 2007
 CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(6-chloro-7-hydroxy-5-methylpyrazolo[1,5-a]pyrimidin-2-yl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)
 FS STEREOSEARCH
 MF C28 H31 Cl N6 O4
 SR CA
 LC STN Files: CA, CAPLUS

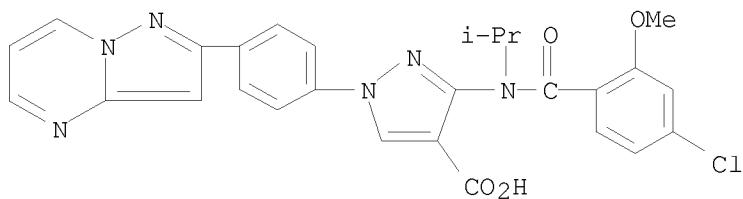
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 5 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 934333-09-2 REGISTRY
 ED Entered STN: 06 May 2007
 CN 1H-Pyrazole-4-carboxylic acid, 3-[(4-chloro-2-methoxybenzoyl)(1-methylethyl)amino]-1-(4-pyrazolo[1,5-a]pyrimidin-2-ylphenyl)- (CA INDEX NAME)
 OTHER NAMES:
 CN 3-[[4-Chloro-2-(methyloxy)phenyl]carbonyl](1-methylethyl)amino]-1-[4-(pyrazolo[1,5-a]pyrimidin-2-yl)phenyl]-1H-pyrazole-4-carboxylic acid
 MF C27 H23 Cl N6 O4
 SR CA
 LC STN Files: CA, CAPLUS

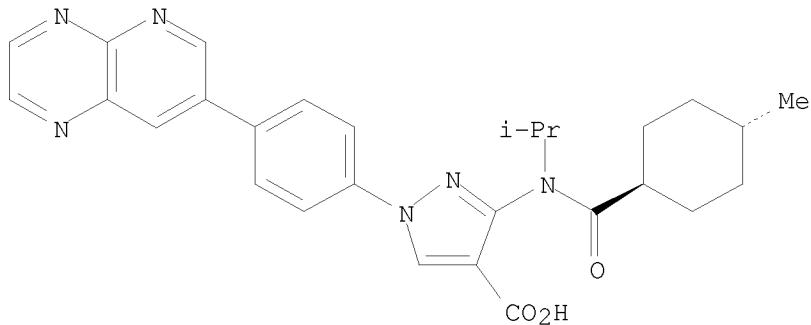


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1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 6 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 934333-08-1 REGISTRY
 ED Entered STN: 06 May 2007
 CN 1H-Pyrazole-4-carboxylic acid, 3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1-(4-pyrido[2,3-b]pyrazin-7-ylphenyl)- (CA INDEX NAME)
 OTHER NAMES:
 CN 3-[(trans-4-Methylcyclohexyl)carbonyl](1-methylethyl)amino]-1-[4-(pyrido[2,3-b]pyrazin-7-yl)phenyl]-1H-pyrazole-4-carboxylic acid
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 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.

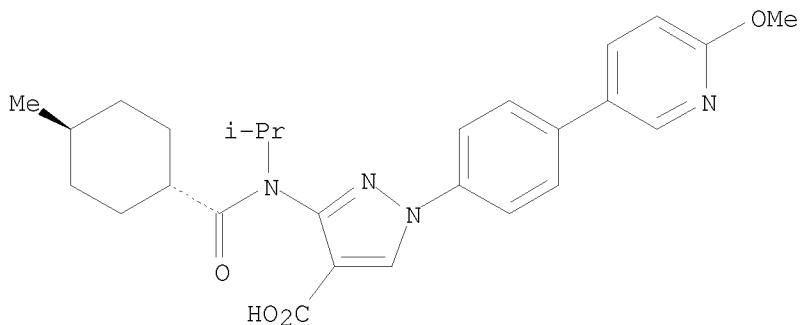


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 7 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 934333-07-0 REGISTRY
 ED Entered STN: 06 May 2007
 CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(6-methoxy-3-pyridinyl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)
 OTHER NAMES:
 CN 3-[(trans-4-Methylcyclohexyl)carbonyl](1-methylethyl)amino]-1-[4-(6-methoxy-3-pyridinyl)phenyl]-1H-pyrazole-4-carboxylic acid
 FS STEREOSEARCH
 MF C27 H32 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 8 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 934333-06-9 REGISTRY

ED Entered STN: 06 May 2007

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(6-acetyl-3-pyridinyl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

OTHER NAMES:

CN 1-[4-(6-Acetyl-3-pyridinyl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1H-pyrazole-4-carboxylic acid

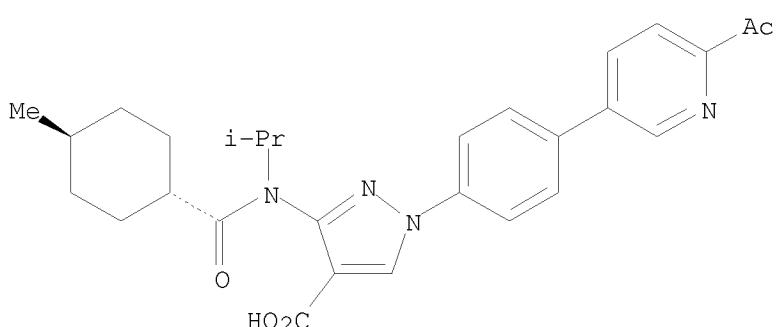
FS STEREOSEARCH

MF C28 H32 N4 O4

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.



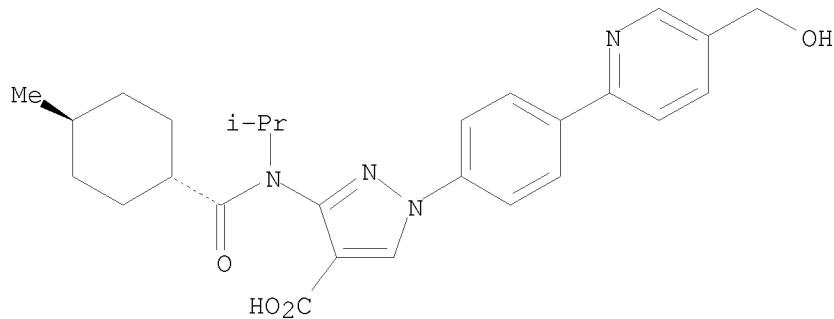
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1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 9 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 934333-05-8 REGISTRY

ED Entered STN: 06 May 2007
 CN 1H-Pyrazole-4-carboxylic acid, 1-[4-[5-(hydroxymethyl)-2-pyridinyl]phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)
 OTHER NAMES:
 CN 1-[4-[5-(Hydroxymethyl)-2-pyridinyl]phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1H-pyrazole-4-carboxylic acid
 FS STEREOSEARCH
 MF C27 H32 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.

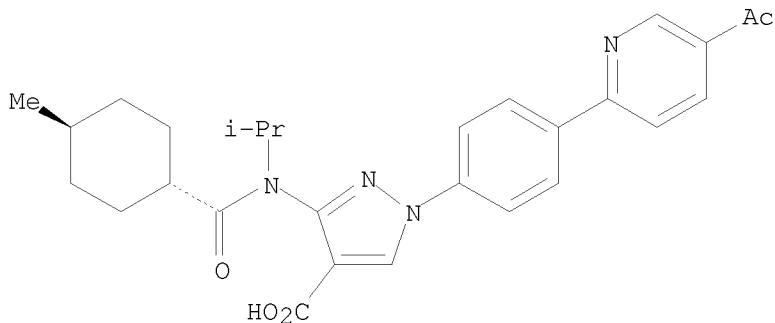


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 10 OF 331 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 934333-04-7 REGISTRY
 ED Entered STN: 06 May 2007
 CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(5-acetyl-2-pyridinyl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)
 OTHER NAMES:
 CN 1-[4-(5-Acetyl-2-pyridinyl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1H-pyrazole-4-carboxylic acid
 FS STEREOSEARCH
 MF C28 H32 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
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FILE COVERS 1907 - 17 Mar 2009 VOL 150 ISS 12
 FILE LAST UPDATED: 16 Mar 2009 (20090316/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

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 L3 2 L2

=> d 13 1-2 ibib abs hitstr

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2007:409486 CAPLUS <<LOGINID::20090317>>
 DOCUMENT NUMBER: 146:421977
 TITLE: Preparation of 4-carboxypyrazoles as antivirals for
 treatment of hepatitis C virus (HCV) infection
 INVENTOR(S): Bravi, Gianpaolo; Cheasty, Anne Goretti; Corfield,
 John Andrew; Grimes, Richard Martin; Harrison, David;
 Hartley, Charles David; Howes, Peter David; Medhurst,
 Katrina Jane; Meeson, Malcolm Lees; Mordaunt,
 Jacqueline Elizabeth; Shah, Pritom; Slater, Martin
 John; White, Gemma Victoria
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
 SOURCE: PCT Int. Appl., 275pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

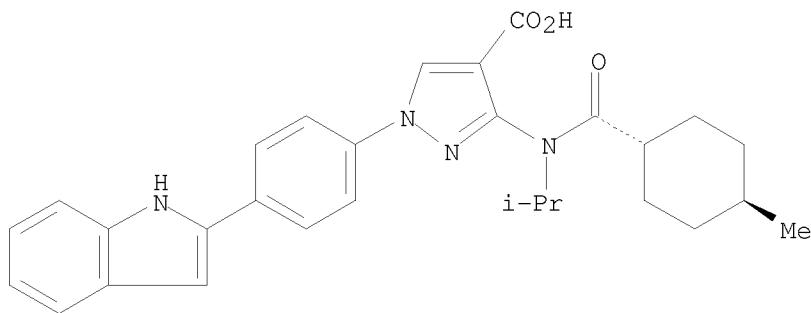
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007039146	A1	20070412	WO 2006-EP9238	20060921
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:			GB 2005-19474	A 20050923
			GB 2006-5467	A 20060317

OTHER SOURCE(S): MARPAT 146:421977
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R1 = -Rx-Ry; Rx = (un)substituted phenylene, or 5- to
 6-membered heteroarylene bonded through a ring C to the N of the pyrazole;
 Ry = heteroaryl, bonded such that when Rx = Ph, Ry is in the
 para-position; R2 = Ph, cycloalkyl, cycloalkylmethyl; R3 = heterocyclyl,
 (un)substituted Ph, alkyl; and their salts, solvates and esters], were
 prepared for treating hepatitis C virus (HCV) infection. Thus, a multi-step
 synthesis from Et 3-amino-1H-pyrazole-4-carboxylate via Et
 3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1H-pyrazole-4-
 carboxylate (preparation given) was provided for carboxypyrazole II. I
 inhibited HCV RNA-dependent RNA polymerase with IC50 <10 nM.
 RN 934331-05-2 CAPLUS
 CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(1H-indol-2-yl)phenyl]-3-[(trans-4-
 methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

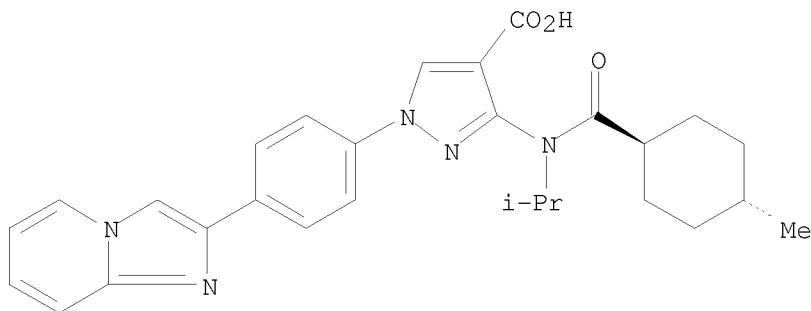
Relative stereochemistry.



RN 934331-06-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(4-imidazo[1,2-a]pyridin-2-ylphenyl)-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

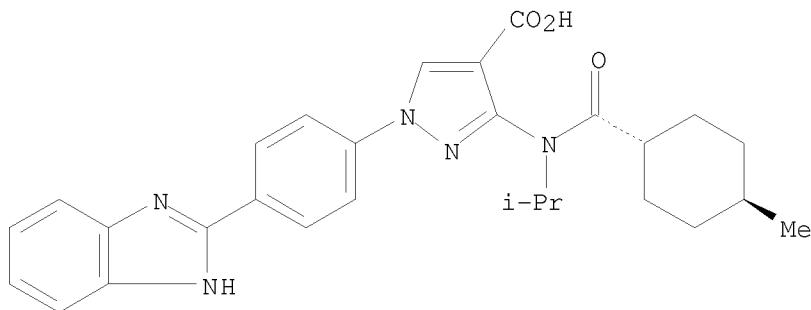
Relative stereochemistry.



RN 934331-07-4 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(1H-benzimidazol-2-yl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

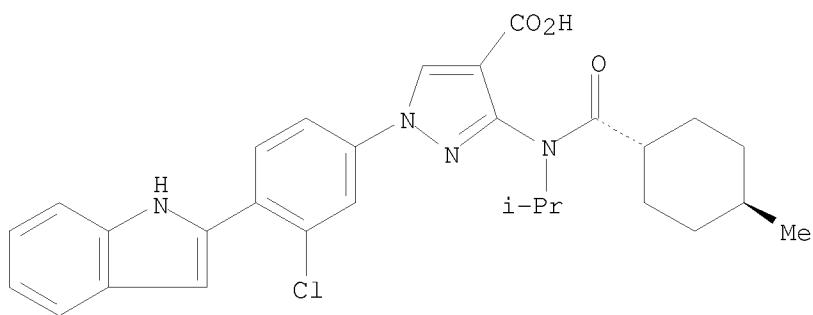
Relative stereochemistry.



RN 934331-08-5 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[3-chloro-4-(1H-indol-2-yl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

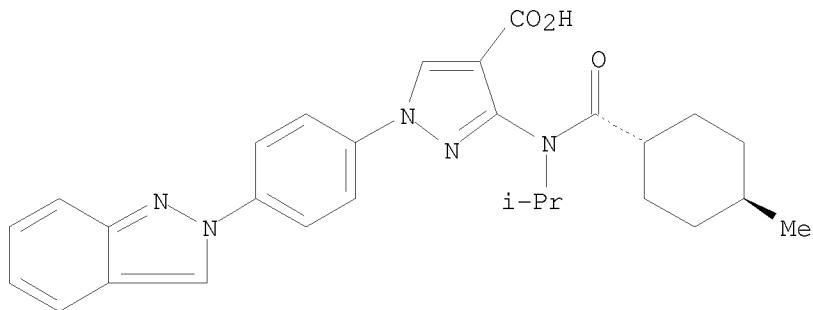
Relative stereochemistry.



RN 934331-09-6 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(2H-indazol-2-yl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

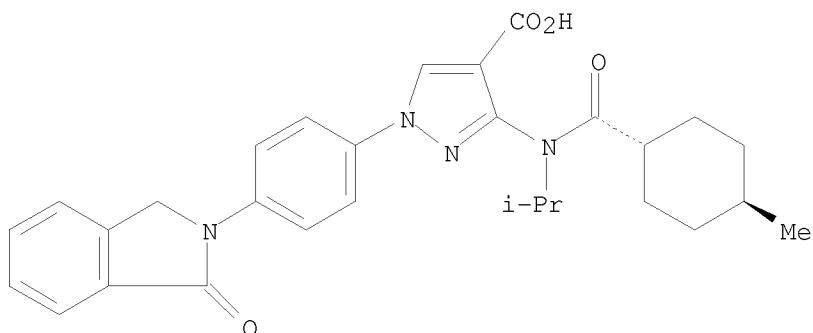
Relative stereochemistry.



RN 934331-10-9 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(1,3-dihydro-1-oxo-2H-isoindol-2-yl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

Relative stereochemistry.

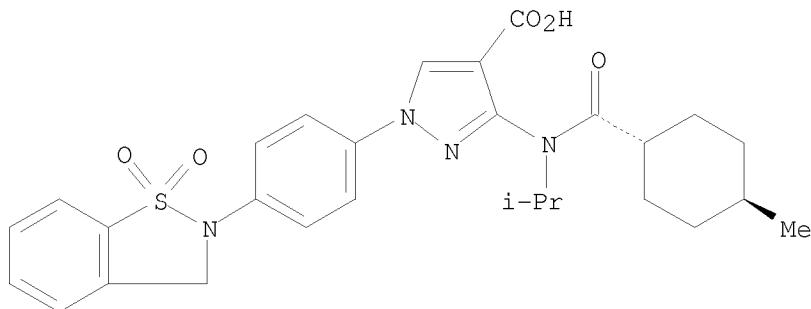


RN 934331-11-0 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(1,1-dioxido-1,2-benzisothiazol-2(3H)-yl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-

(CA INDEX NAME)

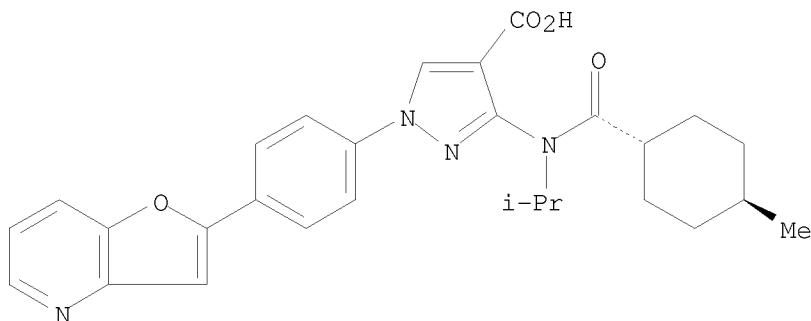
Relative stereochemistry.



RN 934331-12-1 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[4-furo[3,2-b]pyridin-2-ylphenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

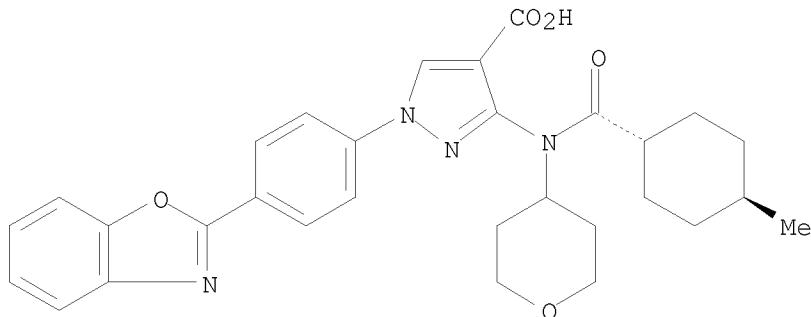
Relative stereochemistry.



RN 934331-13-2 CAPLUS

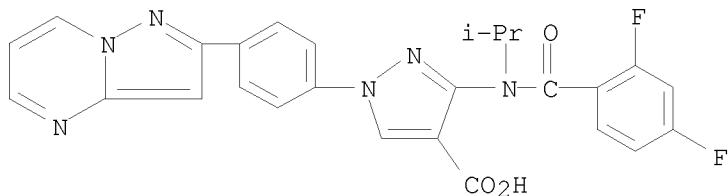
CN 1H-Pyrazole-4-carboxylic acid, 1-[4-(2-benzoxazolyl)phenyl]-3-[(trans-4-methylcyclohexyl)carbonyl](tetrahydro-2H-pyran-4-yl)amino]- (CA INDEX NAME)

Relative stereochemistry.



RN 934333-11-6 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[(2,4-difluorobenzoyl)(1-methylethyl)amino]-1-(4-pyrazolo[1,5-a]pyrimidin-2-ylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

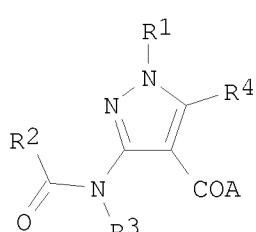
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1075778 CAPLUS <<LOGINID::20090317>>
DOCUMENT NUMBER: 143:347168
TITLE: Preparation of pyrazole-4-carboxylic acids as HCV RNA polymerase inhibitors for the treatment of viral infections
INVENTOR(S): Bravi, Gianpaolo; Corfield, John Andrew; Grimes, Richard Martin; Guidetti, Rossella; Lovegrove, Victoria Lucy Helen; Mordaunt, Jacqueline Elizabeth; Shah, Pritom; Slater, Martin John
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 140 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005092863	A1	20051006	WO 2005-GB1071	20050322
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EP 1730116	A1	20061213	EP 2005-729380	20050322
EP 1730116	B1	20070905		
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CN 1960976	A	20070509	CN 2005-80017114	20050322
AT 372323	T	20070915	AT 2005-729380	20050322
JP 2007530516	T	20071101	JP 2007-504463	20050322
ES 2292126	T3	20080301	ES 2005-729380	20050322
IN 2006DN05138	A	20070803	IN 2006-DN5138	20060906
US 20070167507	A1	20070719	US 2006-599346	20060926
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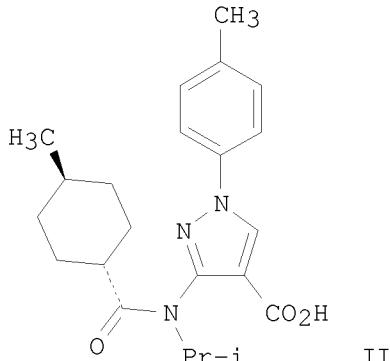
GB 2004-6918	A 20040326
GB 2004-23000	A 20041015
GB 2004-23001	A 20041015
WO 2005-GB1071	W 20050322

OTHER SOURCE(S):
GI

CASREACT 143:347168; MARPAT 143:347168



I



II

AB The invention relates to the title compds. I [wherein A = OH; R1 = (un)substituted (hetero)aryl or heterocyclyl; R2 = substituted Ph or (un)substituted cycloalkyl(methyl); R3 = (un)substituted heterocyclyl, heteroaryl, Ph or alkyl; R4 = H, and salts, solvates and esters thereof], a process for their preps. and use as antiviral agents. For instance, acid II was synthesized by hydrolysis of the corresponding Et ester (preparation given) with LiOH in THF-EtOH at rt for 16 h. Exemplified compds. I (no indication) had inhibition against HCV RNA-dependent RNA polymerase with IC₅₀ values of <80 μM. Therefore, I and their pharmaceutical compns. are useful as HCV RNA polymerase inhibitors and in treating and/or preventing viral infections.

IT 865870-39-9P

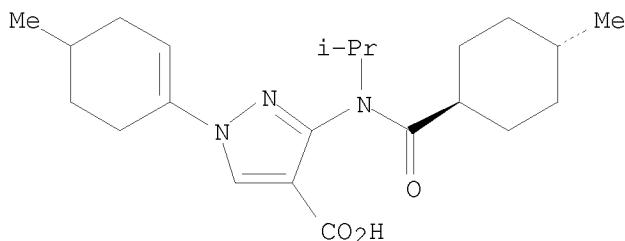
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrazolecarboxylic acids as HCV RNA polymerase inhibitors for the treatment of viral infections)

RN 865870-39-9 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(4-methyl-1-cyclohexen-1-yl)-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

Relative stereochemistry.



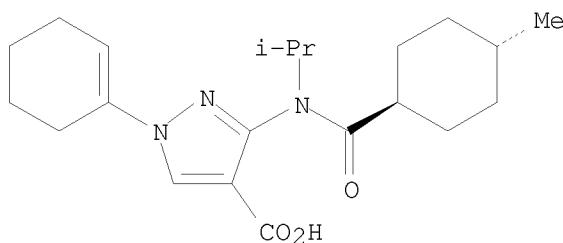
IT 865869-73-4P 865870-69-5P 865870-90-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrazolecarboxylic acids as HCV RNA polymerase inhibitors for the treatment of viral infections)

RN 865869-73-4 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(1-cyclohexen-1-yl)-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

Relative stereochemistry.

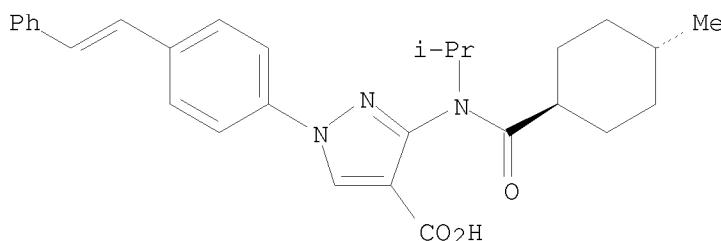


RN 865870-69-5 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1-[4-(2-phenylethenyl)phenyl]- (CA INDEX NAME)

Relative stereochemistry.

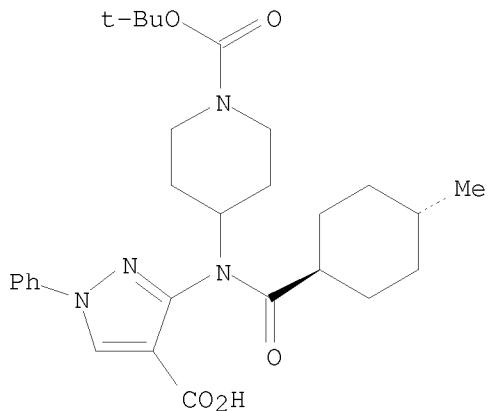
Double bond geometry unknown.



RN 865870-90-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[(4-carboxy-1-phenyl-1H-pyrazol-3-yl)[(trans-4-methylcyclohexyl)carbonyl]amino]-, 1-(1,1-dimethylethyl)ester (CA INDEX NAME)

Relative stereochemistry.



IT 865869-71-2P 865869-72-3P 865869-74-5P
 865869-75-6P 865869-76-7P 865869-77-8P
 865869-78-9P 865869-79-0P 865869-80-3P
 865869-81-4P 865869-82-5P 865869-83-6P
 865869-84-7P 865869-85-8P 865869-86-9P
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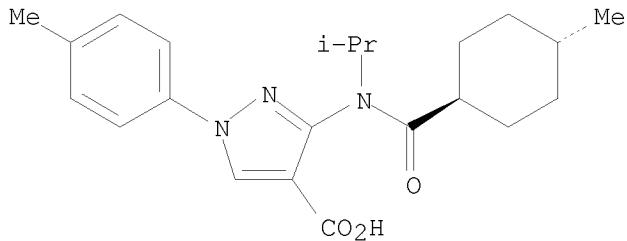
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrazolecarboxylic acids as HCV RNA polymerase inhibitors for the treatment of viral infections)

RN 865869-71-2 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1-(4-methylphenyl)- (CA INDEX NAME)

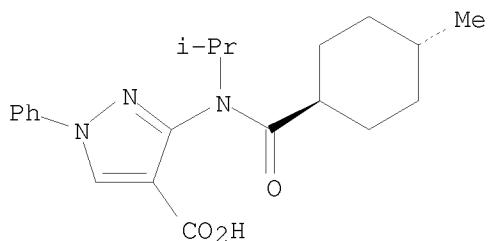
Relative stereochemistry.



RN 865869-72-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]-1-phenyl- (CA INDEX NAME)

Relative stereochemistry.



RN 865869-74-5 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(4-chloro-3-methylphenyl)-3-[(trans-4-methylcyclohexyl)carbonyl](1-methylethyl)amino]- (CA INDEX NAME)

Relative stereochemistry.

